ChemistryOPEN

Supporting Information

Topological Control of Columnar Stacking Made of Liquid-Crystalline Thiophene-Fused Metallonaphthalocyanines

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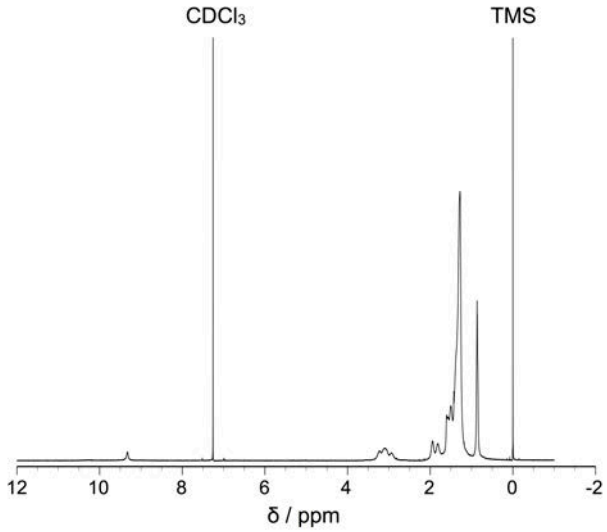
a)



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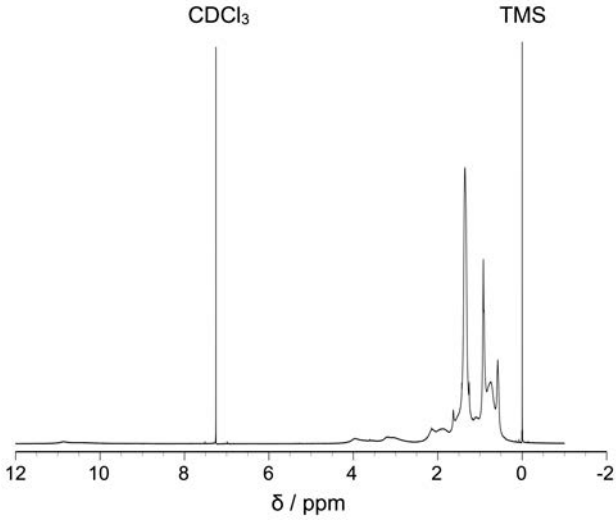
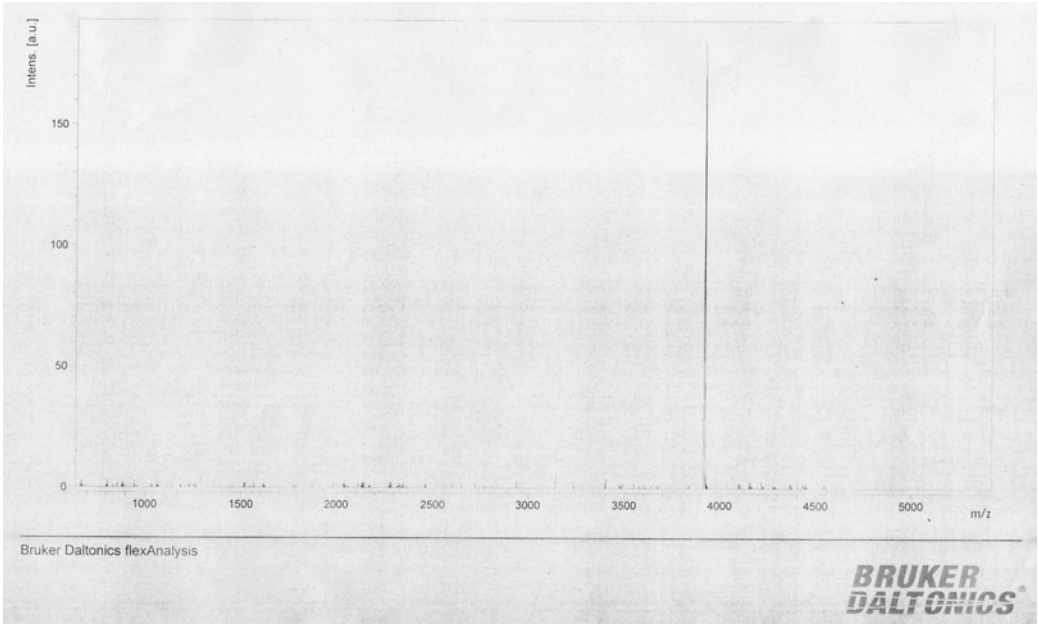


Fig. S1 ^{1}H NMR spectra of a) **ZnTNc$_{endo}$** and b) **ZnTNc$_{exo}$** in $CDCl_3$.

a)



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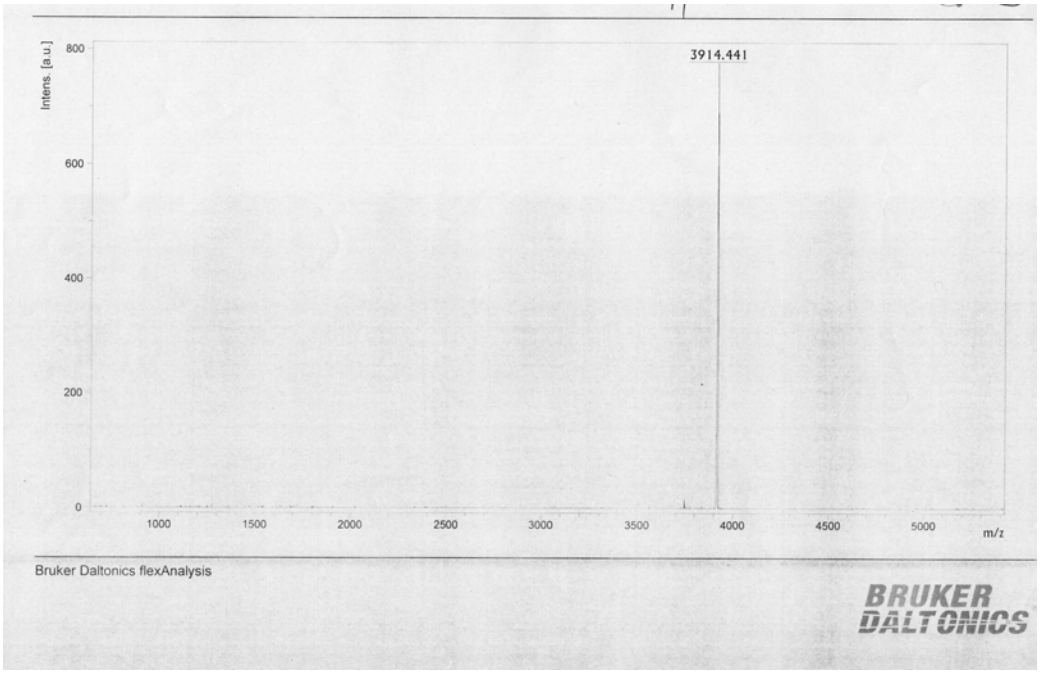

Fig. S2 MALDI-TOF Ms spectra of a) **ZnTNc$_{endo}$** and b) **ZnTNc$_{exo}$**.

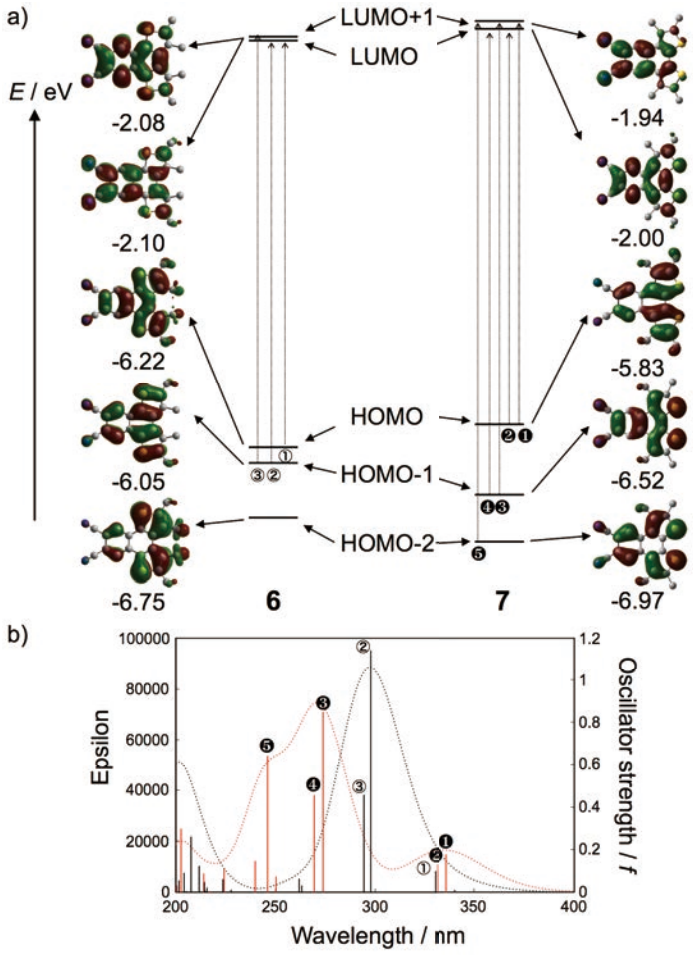

Fig. S3 a) Molecular orbitals and energy diagrams of **6** and **7** (methyl-substituted analogues) obtained by DFT at the B3LYP/6-31G(d) level, respectively. b) Simulated absorption spectra and oscillator strength of **6** (black) and **7** (red) obtained by TD-DFT at the CAM-B3LYP/6-31G(d) level.

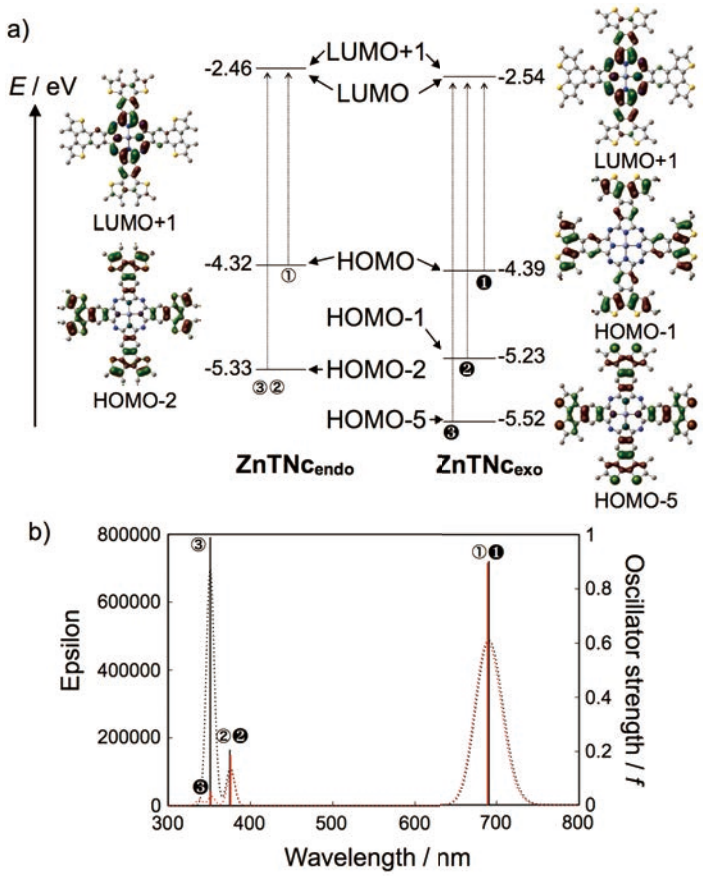

Fig. S4 a) Molecular orbitals and energy diagrams of **ZnTNc$_{endo}$** and **ZnTNc$_{exo}$** (methyl-substituted analogues) obtained by DFT at the B3LYP/6-31G(d) level, respectively. b) Simulated absorption spectra and oscillator strength of **ZnTNc$_{endo}$** (black) and **ZnTNc$_{exo}$** (red) obtained by TD-DFT at the CAM-B3LYP/6-31G(d) level.

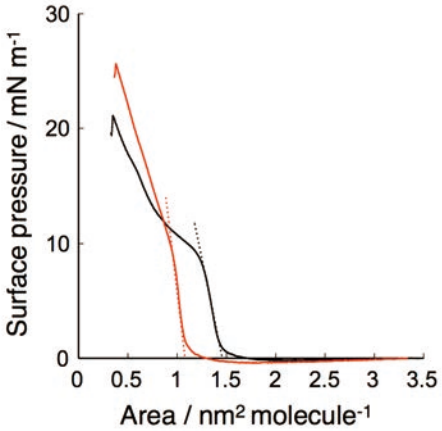

Fig. S5 Surface pressure *vs.* area per molecule isotherms for **ZnTNc$_{endo}$** (black line) and **ZnTNc$_{exo}$** (red line) on triply distilled water at 25 ºC.

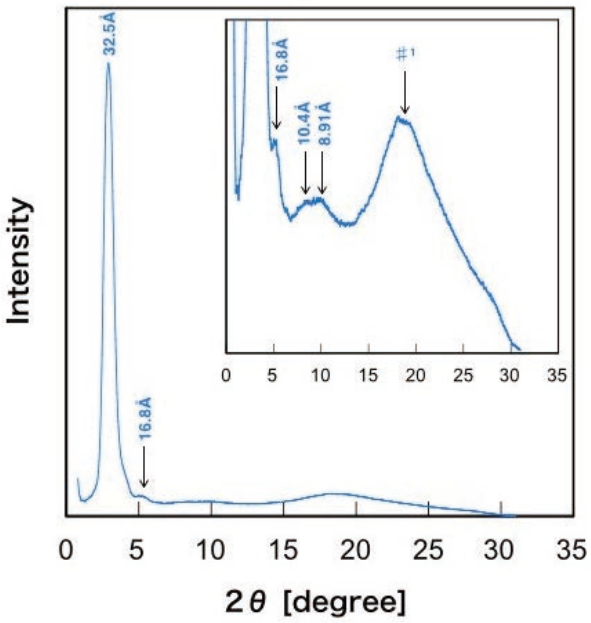

Fig. S6 X-ray diffraction patterns of **ZnTNc$_{endo}$** at 160 ºC.

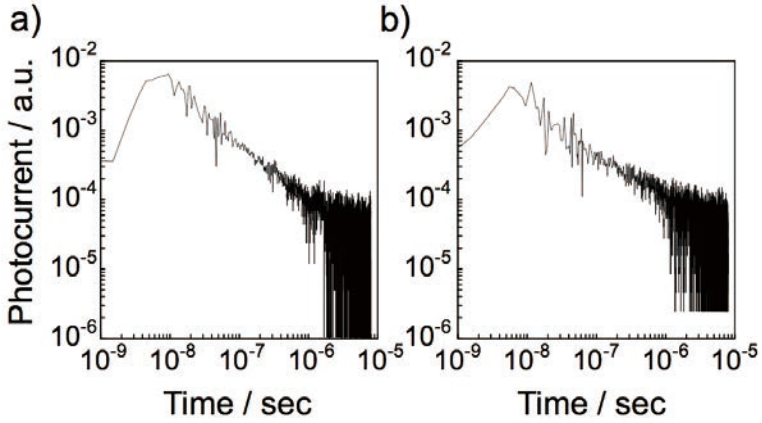

Fig. S7 Photocurrent decay properties for a) positive (bias voltage = -80 V) and b) negative (bias voltage = 80 V) charge carriers of **ZnTNc$_{exo}$** at 150 ºC.